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Spontaneous magnetization in single and coupled quantum dots

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Abstract. Spontaneous magnetization of single and coupled quantum dots formed by lateral confinement of a high-mobility two-dimensional electron gas is studied for a realistic semiconductor heterostructure. The modeling of the device takes into account contributions from a patterned gate, doping, surface states and mirror charges. To explore the magnetic properties we use the Kohn–Sham local spin-density formalism including the contributions from electron correlation as well as from exchange. We show, however, by explicit calulations that the exchange is the dominant mechanism driving a spontaneous magnetization of a dot. Single dots and pairs of dots with up to about 50 electrons per dot have been studied. The question of very large dots is also addressed briefly.

Introduction

The expectations to utilize quantum dots and the inherent magnetic properties in semiconductor electronics are high [1]. There is, for example, the emerging field of spin electronics, or 'spintronics', which takes advantage of electron spin rather than its charge and which may bring about new devices such as spin transistors, magnetic random access memories, and optical encoders and decoders [2]. An even more ambitious application might be in using coherent states of electron spins for quantum information processing. Semiconductor quantum dots are especially attractive for these purposes since their electronic properties can be readily engineered and spin coherence can be sustained long enough to be monitored and transported within the device [3]. Given such a motivation, it is instructive to study single and coupled quantum dots in terms of their magnetization (spin polarization), and how the latter could be controlled by external means.

In this paper we will discuss the self-consistent Kohn–Sham local spin density functional method (LSD) [4] as applied to the calculation of the capacitance and charging energies, i.e., basic parameters of quantum devices containing arrays of ultra-small dots in GaAs/$Al_xGa_{1-x}As$ heterojunction. With this approach, we thus investigate atomic-like shell structures and magnetized states. Details of our work are found in [1, 5].

1. Theoretical modeling

Quantum-dot devices may be fabricated in a semiconductor heterostructure with a patterned metallic top gate [6]. The gate is deposited everywhere on top of the structure except for ungated openings. Dots residing at the interface arise from the depletion of the two-dimensional electron gas (2DEG) under the gated regions when a negative gate voltage is

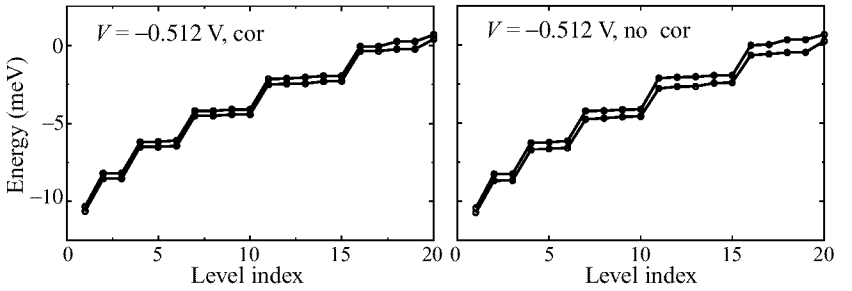

Fig. 1. Spin-split electron levels in a quantum dot at a certain gate voltage V. In the upper case both electron correlation and exhange are included in the Kohn–Sham potential U_{ex}^{σ}, while the lower one includes exchange only. The chemical potential is set to zero, hence there are 19 up-spin and 17 down-spin electrons in the upper case. The corresponding numbers for the lower case are 19 and 16.

applied. The actual size of the dots can be varied by changing the geometry of the gate, i.e. its lithography, as well as the applied gate voltage.

To find the electronic structure, number of electrons in a dot etc. we solve the Kohn–Sham equations by discretizing on a square grid:

$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\varphi^{\sigma}(x,y)+[U(x,y)+U_{ex}^{\sigma}(x,y)]\varphi^{\sigma}(x,y)=E^{\sigma}\varphi^{\sigma}(x,y). \quad (1)$$

Here $\sigma = \pm\frac{1}{2}$ refers to the two spin directions, $U(x, y)$ represents the potential from the electrostatic confinement and the repulsive Hartree term. The important exchange-correlation potential is denoted $U_{ex}^{\sigma}(x, y)$. In the calculations we have used two form for U_{ex}^{σ}, one with both electron correlation and exchange included and one with exchange only.

2. Electronic configurations and spontaneous magnetization

The magnetization (spin polarization) of a dot is defined as the difference between the densities n^{σ} of the up and down-spin electrons

$$p = n^{\uparrow} - n^{\downarrow}. \quad (2)$$

We have simulated a single quantum associated with a symmetric square opening in the gate. At the interface the corresonding potential is in practice circular. We have searched a large gate voltage region yielding 0 to 50 electrons in the dot. The results show a rich variety of magnetizations depending on the number of electrons occupying the dot. Because of the high symmetry there is a pronounced shell structure where the lower shells are filled with both up and down-spin electrons while the uppermost shell may be only partially filled with, let us say, up-spin electrons. The corresponding states for down-spin electrons are above the Fermi level. A typical example is presented in Fig. 1 for a given gate voltage V. The upper case shows the spin-polarised levels with both electron interactions and exchange included in U_{ex}^{σ} while the lower case refers to exchange only. Although the splitting of levels is reduced with correlations included the total spin and shell-filling remain the same as for the case with only exchange. Obviously, correlation also requires slight adjustments of V to have the same number of electrons in the dot.

The overall results for the single symmetric quantum dot are presented in Fig. 2. A Coulomb staircase that is shown to the right reflects the filling of the dot with electrons

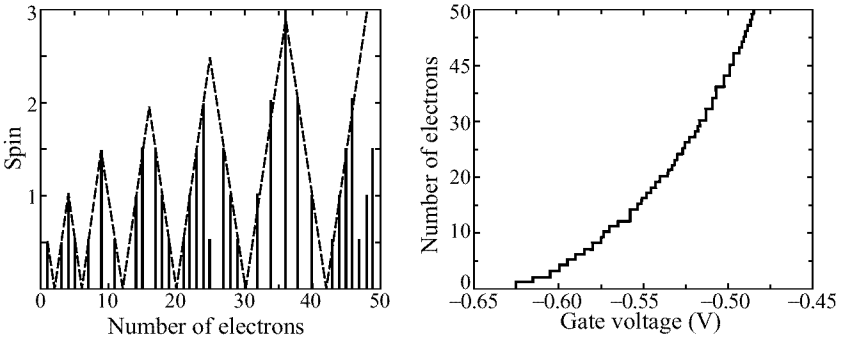

Fig. 2. (a) Coulomb staircase diagram for a single square quantum dot. (b) Variation of the total spin polarization in the square quantum dot containing N_{tot} electrons. Solid bars represent the results of the modeling. The dashed line indicates the spin configuration when Hund's rule is satisfied.

as a function of the gate voltage. The total number of electrons varies from 0 at a pinch-off voltage of -0.62 V and up to 50 electrons. Some of the steps along the vertical axis experience a jump of two electrons (such as from 12 to 14 and in the region from 30 to 42 electrons). In those cases the step of the gate voltage $\Delta V_g = 1$ mV has not been sufficiently small to distinguish between a pair of highly degenerate energy states, and a double filling has occurred.

The left part of Fig. 2 plots the total spin polarization S_z of the dot as a function of its electron content. In general, by external variations in the gate voltage one can vary the spin polarization (magnetization) of a single symmetric quantum dot in a range limited by Hund's rule. This is as long as the dot has circular symmetry. If we introduce a dent by applying different voltages to different segments of the gate the shell structure breaks down and the magnetization is removed. In the same way we find that the magnetization is stongly affected when two dots are made to interact. This gives in principle a way to control the magnetization. Presently we are extending this considerations to very large dots with up to 1000 electrons for which our methos is well suited. In this way we plan make contact with current measurements of the magnetization of dots.

References

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